# AB INITIO STUDY OF DECAY WIDTHS AND BRANCHING RATIOS OF NEUTRON RESONANCES OF LIGHT NUCLEI

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# Ab initio calculations of light nuclei using NCSM

The formalism of No-Core Shell Model (NCSM) is following:

1) Basis components are

$$\psi_{i} = \begin{vmatrix} \psi_{n_{1}l_{1}j_{1}m_{1}}(r_{1}) & \dots & \psi_{n_{A}l_{A}j_{A}m_{A}}(r_{1}) \\ \dots & \dots & \dots \\ \psi_{n_{1}l_{1}j_{1}m_{1}}(r_{A}) & \dots & \psi_{n_{A}l_{A}j_{A}m_{A}}(r_{A}) \end{vmatrix}.$$
(1)

The basis limit is  $\sum_{k=1}^{A} 2n_k + l_k \leq N_{\max}^{sum}$ .

2) The A-nucleon Schrödinger equation is solved on the built basis  $H\psi = E\psi, \psi = \sum_i c_i \psi_i, H = T + U$ 

3) The solution of the equation is equal to the calculation of lowest eigenvalues of the following matrix

$$\begin{vmatrix} \langle \psi_1 | H | \psi_1 \rangle & \dots & \langle \psi_N | H | \psi_1 \rangle \\ \dots & \dots & \dots \\ \langle \psi_1 | H | \psi_N \rangle & \dots & \langle \psi_N | H | \psi_N \rangle \end{vmatrix}$$

The dimension of the Slater determinants basis is up to 10<sup>10</sup> on modern supercomputers.

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4) Calculation method is iterative Lanczos algorithm for eigenvalues and eigenvectors usually.

5) The results are total binding energies and wave functions of the ground and lower exited states of light nuclei obtained in ab initio calculations.

**DISADVANTAGES:** Difficulties in calculations of the asymptotic characteristics of various nucleon and cluster channels (it means difficulties with decay widths and cross sections) due to extremely growth of SD basis.





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### Cluster Channel Orthogonal Functions Model (CCOFM)

CCOFM model could be used for ab initio calculations of various nuclear characteristics:



Ab initio nuclear spectra calculations in clustered and combined bases Calculations of cluster and asymptotic properties of ground and lower exited states:

- 1) spectroscopic factors
- 2) nucleon and cluster formfactors
- 3) partial decay widths of resonances
- 4) asymptotic normalizing coefficients of bound states



#### Construction of cluster terms of CCOFM basis

The cluster-channel terms are built in the form of translationally-invariant Anucleon wavefunctions

$$\Psi_{A}^{i} = \frac{1}{W} A \{ \Psi_{A_{1}} \Psi_{A_{2}} \varphi_{nlm}(\rho) \}_{JM_{J}},$$

For ab initio calculations cluster-channel terms must be expressed in the form of Slater determinant superposition:

$$\Psi^{i}_{A} = \sum_{j=1}^{N_{size}} C^{i}_{j} \psi_{j}, N_{size} < N^{\max}_{NCSM}$$

The algorithm for construction of the basis WF:

 $\Phi_{000}^{A_i}(R_i)\Psi_{A_i}$  - NCSM solutions for individual clusters with zero vibrations along the coordinate of the center of mass.

Calculations of cluster WF with nonzero vibrations along the coordinate of the center of mass  $\Phi_{NLM}^{A_i}(R_i)\Psi_{A_i}$  as SD superpositions using cluster coefficients method.

Obtaining cluster-channel terms by Talmi-Moshinsky transformation.

$$\mathbf{\Phi}^{i}_{A} = \frac{1}{W} A \left\{ \sum_{N_{1}, L_{1}, M_{1}, N_{2}, L_{2}, M_{2}} \begin{pmatrix} 000 & N_{1}, L_{1}, M_{1} \\ N_{1}, L_{1}, M_{1} \end{pmatrix} \Phi^{A_{1}}_{N_{1}, L_{1}, M_{1}}(R_{1}) \Psi_{A_{1}} \Phi^{A_{2}}_{N_{2}, L_{2}, M_{2}}(R_{2}) \Psi_{A_{2}} \right\}.$$

#### The algorithm of cluster properties calculation



3) Orthogonalization of basis WF for each channel

$$\Psi_{A}^{i} = A\{\{\Psi_{A_{1}}^{J_{1}M_{1}}\Psi_{A_{2}}^{J_{2}M_{2}}\}_{SM_{S}}\varphi_{ilm}(\rho)\}_{JM_{J}}, \varphi_{ilm}(\rho) = \sum_{n} B_{n}^{i}\varphi_{nlm}(\rho)$$

4) The cluster formfactor of fragmentation of the A-nucleon state characterized by the wavefunction  $\Psi_{\it base}$  into this channel has the form

$$F_{l}(r) = \sum_{i} \frac{1}{\sqrt{\varepsilon_{i}}} \left\langle \Psi_{A}^{i} \right| \Psi_{base} \right\rangle \varphi_{il}(r),$$

5) Obtaining the cluster formfactor as a superposition of oscillator functions and spectroscopic factor, as its normalization.

$$F_l(r) = \sum_n A_n^l \varphi_{nl}(r), \quad A_n^l = \sum_{i,n'} \left( \varepsilon_i \right)^{-1/2} \left\langle \Psi_{base} \left| \Psi_A^{n'lJ_1J_2SJ} \right\rangle B_n^i B_{n'}^i \right\rangle$$

### Calculation of asymptotic properties

1) Narrow neutron resonances calculations

In this case, in a sufficiently wide subbarrier region, nuclear attraction is negligible.

For all this region the relation  $n_l(\mathbf{r}) >> j_l(\mathbf{r})$  takes place.

It means that regular function could be neglected.

To determine the position of the matching point  $R_{point}$  of the cluster formfactor and irregular wavefunction in this range,  $\frac{F'_l(r)}{F_l(r)} = \frac{n'_l(r)}{n_l(r)}$ . we use the condition of equality of the logarithmic  $\frac{F'_l(r)}{F_l(r)} = \frac{n'_l(r)}{n_l(r)}$ . derivatives:

Therefore, the decay width of the neutron  $\ \Gamma =$  resonance is given by the expression:

$$\frac{h^2}{\mu k} \left( \frac{F_l(R_{point})}{n_l(R_{point})} \right)^2$$

2) Proton and cluster resonances calculations

For proton and cluster resonances Coulomb functions are used instead of Neiman and Bessel functions.

3) Calculations of asymptotic normalizing coefficients of bound states

$$ANC = \frac{rF_l(r)}{W_{-\eta,l+1/2}(2kr)}$$



#### **Calculation results**

For ab initio calculations of light nuclei properties, modern realistic NN-potentials Daejeon16 and JISP16 were used. These universal potentials describe the spectra of all light nuclei up to <sup>16</sup>O without additional phenomenological parameters.

For the oscillator basis, the distance region, where the solutions of the Schrödinger equation are described correctly, expands in proportion to  $[N_{max}^{tot}]^{1/2}$ . In this connection, a microscopic description of cluster channels at distances where asymptotic representation is correct requires an extremely large NCSM basis.

Therefore, the cutoff parameter for the <sup>7</sup>Li basis is 16, and the corresponding SD basis is 5.1 \* 10<sup>8</sup>, in the case of the <sup>5</sup>He, the cutoff parameter is 17.



# Total binding energies of <sup>7</sup>Li, <sup>5</sup>He and their subsystems

Calculations of ground states of <sup>7</sup>Li and <sup>5</sup>He were held for cutoff parameters N<sup>max</sup> = 16 (17) for different values of oscillator parameter  $\hbar \omega$ . Subsystems <sup>4</sup>He, <sup>3</sup>H, <sup>6</sup>Li were calculated with cutoff parameter N<sup>max</sup> = 4.

| Total binding energies of <sup>7</sup> Li, <sup>5</sup> He, <sup>4</sup> He, <sup>3</sup> H, <sup>6</sup> Li. |                     |                   |                     |        |                     |         |        |  |
|---|---------------------|-------------------|---------------------|--------|---------------------|---------|--------|--|
|   | $\hbar\omega$ =12.5 | $\hbar\omega$ =15 | $\hbar\omega$ =17.5 | ħω =20 | $\hbar\omega$ =22.5 | ħω =25  | exp.   |  |
| <sup>5</sup> He   | 27.335              | 27.279            | 27.209              |        |                     |         | 27.41  |  |
| <sup>7</sup> Li   |                     |                   |                     | 39.110 | 38.909              | 38.620  | 39.245 |  |
| ⁴He   | 26.778              | 27.784            | 28.102              | 28.158 | 28.126              | 28.051  | 28.296 |  |
| %(0s1/2 <sup>4</sup> )  | 0.891               | 0.9373            | 0.9694              | 0.9848 | 0.9861              | 0.97724 |        |  |
| <sup>3</sup> Н  |                     |                   |                     | 7.976  | 7.802               | 7.598   | 8.482  |  |
| %(0s1/2 <sup>3</sup> )  |                     |                   |                     | 0.9740 | 0.9628              | 0.9489  |        |  |
| <sup>6</sup> Li   |                     |                   |                     | 29.186 | 28.409              | 27.325  | 31.995 |  |

For given basis cutoff parameters, the ground states of <sup>7</sup>Li and <sup>5</sup>He and their subsystems <sup>4</sup>He, <sup>3</sup>H, <sup>6</sup>Li are described with good accuracy.





Function of neutron formfactor  $3/2^-$  turns out to be stable with respect to changes in the accuracy of description of <sup>4</sup>He and changes in oscillator parameter  $\hbar\omega$ .

For the value of the energy of the given resonance ( $E_{exp}$  = 27.4 MeV,  $E_{res}$  = 0.890 MeV) in the all region of interest to us along the coordinate r  $n_l(r) >> j_l(r)$ .

In this case  $P_l(r) \approx (kr)^{-2} (n_l(r))^{-2}$ .







Logarithmic derivatives of neutron formfactors and Neiman function,  $\hbar \omega$  = 17.5 MeV.

As follows from the ratio between the asymptotic solution and the neutron formfactor, the ab initio calculations accurately describe the asymptotic region.





#### The results of the calculation of the width of 3/2<sup>-</sup> resonance <sup>5</sup>He

Calculations of the 3/2<sup>-5</sup>He state were carried out for a wide range of NCSM bases cutoff parameters for <sup>5</sup>He (N<sub>max</sub>) and <sup>4</sup>He (N<sub>He</sub>) and the oscillatory parameter  $\hbar \omega$ . The results are shown in the table. The experimental value of the resonance width is 600 keV.

| Decay width of 3/2- 5He |  |                                 |  |                                   |                                 |                                   |  |                                 |                                   |
|-------------------------|--|---------------------------------|--|-----------------------------------|---------------------------------|-----------------------------------|--|---------------------------------|-----------------------------------|
|                         | $N_{max}$ =13<br>$\hbar \omega$ = 12.5 | N <sub>max</sub> =13<br>ħ∞ = 15 | $N_{max}$ =13<br>$\hbar \omega$ = 17.5 | N <sub>max</sub> =15<br>ħω = 12.5 | N <sub>max</sub> =15<br>ħω = 15 | N <sub>max</sub> =15<br>ħω = 17.5 | $N_{max}$ =17<br>$\hbar \omega$ = 12.5 | N <sub>max</sub> =17<br>ħω = 15 | N <sub>max</sub> =17<br>ħω = 17.5 |
| N <sub>He</sub> = 0     | 469 кэВ                                | 548 кэВ                         | 628 кэВ                                | 443 кэВ                           | 530 кэВ                         | 597 кэВ                           | 427 кэВ                                | 578 кэВ                         | 577 кэВ                           |
| N <sub>He</sub> = 2     | 545 кэВ                                | 588 кэВ                         | 625 кэВ                                | 545 кэВ                           | 590 кэВ                         | 615 кэВ                           | 515 кэВ                                | 587 кэВ                         | 600 кэВ                           |
| N <sub>He</sub> = 4     | 642 кэВ                                | 678 кэВ                         | 642 кэВ                                | 563 кэВ                           | 629 кэВ                         | 630 кэВ                           |  | 611 кэВ                         | 620 кэВ                           |

Theoretical calculations show good agreement with experiment and stability with respect to changing free parameters of the basis.





### Calculations of ground and exited states of <sup>7</sup>Li

| Spectrum of lowest states of <sup>7</sup> Li |          |     |          |                                    |                        |  |
|--|----------|-----|----------|------------------------------------|------------------------|--|
|  | exp. (E) | Т   | Г (ехр.) | $\hbar\omega$ =20 (E)<br>Daejeon16 | ħω =22.5 (E)<br>JISP16 |  |
| 3/2⁻   | 39.245   | 1/2 |          | 39.110                             | 37.929                 |  |
| 1/2⁻   | 38.788   | 1/2 | 73 fs    | 38.279                             | 37.290                 |  |
| 7/2-   | 34.615   | 1/2 | 93 keV   | 34.410                             | 32.625                 |  |
| 5/2⁻   | 32.565   | 1/2 | 880 keV  | 31.613                             | 30.332                 |  |
| 5/2-   | 31.786   | 1/2 | 89 keV   | 30.816                             | 29.491                 |  |
| 7/2-   | 29.575   | 1/2 | 400 keV  | 28.489                             | 26.840                 |  |
| 3/2⁻   | 29.335   | 1/2 | 1200 keV | 28.175                             | 27.286                 |  |
| 3/2-   | 28.000   | 3/2 | 260 keV  | 27.248                             | 25.383                 |  |

The spectrum of calculated levels shows good agreement with the experiment. This means that these wavefunctions can be used to calculate the partial decay widths of resonances and the asymptotic normalization coefficients of the bound states.





#### **Results of calculations of ANC**

|  | exp.                   | theor. | Daejeon16 | JISP16  |
|--|------------------------|--------|-----------|---------|
| 3/2-: <sup>4</sup> He+ <sup>3</sup> T channel                  | 3.57+-0.15             |        | 3.44      | 2.84    |
| 3/2 <sup>-</sup> : <sup>6</sup> Li+n channel with I=1<br>j=1/2 | ANC <sup>2</sup> =1.22 | 1.652  | -1.6168   | -1.4114 |
| 3/2 <sup>-</sup> : <sup>6</sup> Li+n channel with I=1<br>j=3/2 | ANC <sup>2</sup> =1.66 | 1.890  | 1.317     | 1.1986  |

| 1/2-: channel <sup>4</sup> He+ <sup>3</sup> T                  | 3.0+-0.15 |        | 2.95   | 2.42    |
|--|-----------|--------|--------|---------|
| 1/2 <sup>-</sup> : channel <sup>6</sup> Li+n with I=1<br>j=1/2 |           | -0.543 | -0.531 | -0.3629 |
| 1/2 <sup>-</sup> : channel <sup>6</sup> Li+n with I=1<br>j=3/2 |           | -2.543 | 1.979  | 1.637   |

Theoretical calculations show agreement with the application of realistic potentials based on different principles - Daejeon16 and JISP16, and in the case of the <sup>4</sup>He + <sup>3</sup>T channel show good agreement with the experiment.



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# ANC and partial decay widths of highly excited states <sup>7</sup>Li

|  | exp.               | Daejeon16 | JISP16    |
|--|--------------------|-----------|-----------|
| 7/2 <sup>-</sup> : <sup>4</sup> He+ <sup>3</sup> T channel (Gamma)     | 92 (69) keV        | 65 keV    | 34.8 keV  |
| 7/2-: <sup>6</sup> Li+n channel with I=3 s=1/2 (ANC)                   |                    | 0.01356   | 0.0121    |
| 5/2-: <sup>4</sup> He+ <sup>3</sup> T channel (Gamma)                  | 880 (918) keV      | 564 keV   | 438 keV   |
| 5/2-: <sup>6</sup> Li+n channel with I=1 s=3/2 (ANC)                   |                    | 0.199     | 0.033     |
|  |                    |           |           |
| 5/2 <sup>-</sup> (2): <sup>4</sup> He+ <sup>3</sup> T channel (Gamma)  | Total: 89 (80) keV | 797 keV   | 9.7 keV   |
| 5/2 <sup>-</sup> (2): <sup>6</sup> Li+n channel with I=1 s=3/2 (Gamma) | 57 keV             | 53.15 keV | 86.6 keV  |
|  | 1                  |           |           |
| $7/2^{-}(2)$ : <sup>6</sup> Li+n channel with I=3 s=1/2 (Gamma)        |                    | 0.72 keV  | 0.353 keV |
| 7/2 <sup>-</sup> (2): <sup>6</sup> Li+n channel with I=3 s=3/2 (Gamma) |                    | 44.6 eV   | 13.7 eV   |
|  | 1                  |           |           |
| 3/2 <sup>-</sup> (2): <sup>6</sup> Li+n channel with I=1 s=1/2 (Gamma) | 867 keV            | 223 keV   | 48.9 keV  |
| $3/2^{-}(2)$ : <sup>6</sup> Li+n channel with I=1 s=3/2 (Gamma)        |                    | 1.88 MeV  | 1.88 MeV  |



#### Results of calculations for 1/2<sup>+</sup> state of <sup>7</sup>Li



| N*   3/2- state   1/2+ state     9   38.525   27.343     11   38.901   28.921     12   20.110   20.061 | Total binding energies of 3/2 <sup>-</sup> , 1/2 <sup>+</sup> states in NCSM calculations |            |                        |  |  |  |  |
|--|---|------------|------------------------|--|--|--|--|
| 938.52527.3431138.90128.9211230.11020.061  | N*  | 3/2⁻ state | 1/2 <sup>+</sup> state |  |  |  |  |
| 11 38.901 28.921   12 20.110 20.061  | 9   | 38.525     | 27.343                 |  |  |  |  |
| 12 20.110 20.061   | 11  | 38.901     | 28.921                 |  |  |  |  |
| 39.110 30.061  | 13  | 39.110     | 30.061                 |  |  |  |  |

According to work of A. M.

Mukhamedzhanov and R. E. Tribble (Phys. Rev. C Vol. 59 N. 6) the partial width of the subthreshold resonance at E>0 could be expressed throw ANC:

$$\Gamma_{n}^{0}(E) = \frac{\hbar}{\mu_{ab}} \kappa r_{0} r_{l}(E) \frac{W_{-\eta_{0},l+1/2}^{2}(2k_{0}r_{0})}{r_{0}} |C_{ab}|^{2}$$

|  | exp.      | Daejeon16 | JISP16    |
|--|-----------|-----------|-----------|
| <sup>4</sup> He+ <sup>3</sup> T channel ( $\Gamma_{\alpha}$ )            | 3.152 MeV | 7.4 MeV   | 6.96 MeV  |
| <sup>6</sup> Li+n channel with I=0 s=1/2 (ANC)                           |           | 0.595     | 0.544     |
| <sup>6</sup> Li+n channel with I=0 s=1/2 ( $\Gamma_n^0(1 \mathrm{eV})$ ) | 0.295 keV | 0.540 keV | 0.529 keV |



# Conclusions

I. New ab initio multichannel scheme was developed for calculating the asymptotic characteristics of both bound and resonant states, namely the asymptotic normalization coefficients of bound states and partial decay widths of resonant states. This scheme allows to calculate the asymptotic characteristics of several decay channels of the same state of a light nucleus.

II. The asymptotic characteristics of the bound and resonant states of <sup>5</sup>He and <sup>7</sup>Li nuclei were calculated.

III. The theoretical calculation of lowest resonance state 3/2<sup>-</sup> of <sup>5</sup>He shows high-quality agreement with experimental data.

IV. For the <sup>7</sup>Li nucleus, calculations were performed for all experimentally identified states and for various decay channels. These results, in general, show rather good agreement with experimental data.

V. This approach provides possibilities to test universal realistic NN-potentials.



## **THANK YOU FOR YOUR ATTENTION!**



